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Computation of (a,b)-KA Indices of Some Special Graphs

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Abstract: The significance of the (a,b) -KA indices lies on the fact that their special cases, for pertinently chosen values of the parameters a and b, coincide with the vast majority of previously considered vertex based topological indices. In this paper, we computed the (a,b) - KA indices of some special class of graphs such as regular graph (hyper cube graph and generalized petersen graph), cartesian product graph (grid graph, torus graph and cylinder graph), lollipop graph and Harary graph.

Key Words: Molecular descriptors, (a,b)-KA indices, (a,b)-KA coindices.

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§1. Introduction

All the graphs considered here are finite, undirected, connected with no loops and multiple edges. As usual $p=|V|$ and $q=|E|$ denote the number of vertices and edges of a graph $G=(V,E)$, respectively. The edge connecting the vertices u and v will be denoted by uv. Let $d_G(e)$ denote the degree of an edge e in G, which is defined by $d_G(e)=d_G(u)+d_G(v)-2$ with $e=uv$. For graph theoretic terminology and notation not given here we refer the reader to Kulli [15].

Chemical graph theory is a branch of the mathematical chemistry which has an important effect on the development of the chemical sciences. A single number that can be used to characterize some property of the graph of a molecular structure is called a topological index for that graph. There are numerous molecular descriptors, which are also referred to as topological indices, that have found some applications in theoretical chemistry, especially in QSPR/QSAR/QSTR research. For the historical milestones, some applications and mathematical properties of graph theory, we refer to [4, 6, 8, 10, 20, 32].

The first (a,b)-KA index $KA^1_{(a,b)}(G)$, the second (a,b)-KA index $KA^2_{(a,b)}(G)$ and the third (a,b)-KA index $KA^3_{(a,b)}(G)$ of a graph G are defined as

$$KA^1_{(a,b)}(G)=\sum_{uv\in E(G)}[d_G(u)^a+d_G(v)^a]^b,$$

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$$KA^2_{(a,b)}(G) = \sum_{uv\in E(G)} [d_G(u)^a . d_G(v)^a]^b$$

and

$$KA^3_{(a,b)}(G) = \sum_{uv\in E(G)} | d_G(u)^a - d_G(v)^a |^b,$$

where a and b are real numbers.

These (a,b)-KA indices were introduced by Kulli [21] and elaborated in [24].

§2. The Particular Values of a and b in (a,b)-KA Indices

The majority of hitherto studied vertex degree based topological indices are special cases of (a,b)-KA indices, for particular values of real numbers a and b as follows:

(1) $KA^1_{(1,1)}(G) = M_1(G)$, the first Zagreb index, [12].

(2) $KA^2_{(1,1)}(G) = M_2(G)$, the second Zagreb index, [12].

(3) $KA^1_{(-1,1)}(G) = RM_1(G)$, the redefined first Zagreb index, [29].

(4) $KA^1_{(-1,-1)}(G) = RM_2(G)$, the redefined second Zagreb index, [29].

(5) $KA^1_{(2,1)}(G) = F_1(G)$, the first Forgotten index, [5].

(6) $KA^2_{(2,1)}(G) = F_2(G)$, the second Forgotten index, [16].

(7) $KA^1_{(2,2)}(G) = HF_1(G)$, the first hyper Forgotten index, [9].

(8) $KA^1_{(1,2)}(G) = HM_1(G)$, the first hyper Zagreb index, [31].

(9) $KA^2_{(1,2)}(G) = HM_2(G)$, the second hyper Zagreb index, [34].

(10) $KA^1_{(1,-\frac{1}{2})}(G) = \chi(G)$, the sum connectivity index, [35].

(11) $KA^2_{(1,-\frac{1}{2})}(G) = R(G)$, the Randic index, [28].

(12) $KA^2_{(1,\frac{1}{2})}(G) = RR(G)$, the reciprocal Randić index, [15].

(13) $\frac{1}{2}KA^1_{(1,1)}(G) = SK(G)$, the SK-index, [30].

(14) $KA^1_{(2,\frac{1}{2})}(G) = SO(G)$, the Sombor index, [7].

(15) $KA^3_{(1,1)}(G) = Alb(G)$, the Albertson ($M_i(G)$ Minus) index, [1].

(16) $KA^3_{(-1,1)}(G) = M_{in}(G)$, the misbalance indeg index, [33].

(17) $KA^3_{(\frac{1}{2},1)}(G) = M_{ro}(G)$, the misbalance rodeg index, [33].

(18) $KA^3_{(-\frac{1}{2},1)}(G) = M_{ir}(G)$, the misbalance irdeg index, [33].

(19) $KA^3_{(1,2)}(G) = \sigma(G)$, the Sigma index, [11].

(20) $KA^3_{(-2,1)}(G) = M_s(G)$, the misbalance sdeg index, [33].

(21) $KA^3_{(2,1)}(G) = MF(G)$, the minus F-index, [17].

(22) $KA^3_{(2,2)}(G) = \sigma F(G)$, the square F-index (sigma F-index), [17].

(23) $KA^3_{(2,\frac{1}{2})}(G) = RMF_c(G)$, the receiprocal minus F- index, [18].

(24) $KA^3_{(1,b)}(G) = M_i^b(G)$, the general minus index, [19].

(25) $KA^3_{(a,1)}(G) = M_i^a(G)$, the general misbalance deg index, [25].

(26) $KA^3_{(2,b)}(G) = MF^b(G)$, the general minus F- index, [18].

(27) $KA^1_{(1,b)}(G) = M_1^b(G)$, the first general Zagreb index, [26].

(29) $KA^2_{(1,b)}(G) = R^b(G)$, the general Randic index, [3].

(30) $KA^1_{(a,1)}(G) = M_a(G)$, An edge a- Zagreb index, [27].

(31) $KA^1_{(3,1)}(G) = Y(G)$, the Y-index, [2].

(32) $KA^1_{(1,\frac{1}{2})}(G) = N(G)$, the Nirmala index, [22].

(33) $KA^1_{(3,\frac{1}{2})}(G) = D(G)$, the Dharwad index, [23].

§3. Regular Graphs

An r-regular graph is a graph where each vertex has the same degree r. i.e., $d_G(u) = d_G(v) = r$.

Theorem 3.1 *Let G be an r- regular graph with $p \geq 2$ vertices. Then*

(*i*) $KA^1_{(a,b)}(G) = 2^b q r^{ab} = 2^{b-1} p r^{ab+1}$;

(*ii*) $KA^2_{(a,b)}(G) = q r^{2ab} = \frac{1}{2} p r^{2ab+1}$;

(*iii*) $KA^3_{(a,b)}(G) = 0$.

Proof Let G be an r-regular graph with $p \geq 2$ vertices. Since every vertex is of same degree r, we have $2q = pr$.

(*i*) The first (a,b)-KA index is

$$\begin{aligned} KA^1_{(a,b)}(G) &= \sum_{uv \in E(G)} [d_G(u)^a + d_G(v)^a]^b \\ &= \sum_{uv \in E(G)} [r^a + r^a]^b = 2^b q r^{ab} = 2^{b-1} p r^{ab+1}. \end{aligned}$$

(ii) The second (a,b)-KA index is

$$KA^2_{(a,b)}(G) = \sum_{uv\in E(G)} [d_G(u)^a.d_G(v)^a]^b$$
$$= \sum_{uv\in E(G)} [r^a.r^a]^b = qr^{2ab} = \frac{1}{2}pr^{2ab+1}.$$

(iii) The third (a,b)-KA index is

$$KA^3_{(a,b)}(G) = \sum_{uv\in E(G)} |d_G(u)^a - d_G(v)^a|^b$$
$$= \sum_{uv\in E(G)} |r^a - r^a|^b = 0.$$

Thus, the result follows. □

Corollary 3.1 *If cycle C_p with $p \geq 3$ is a 2-regular graph, then*

(i) $KA^1_{(a,b)}(C_p) = 2^{b(1+a)}q$;
(ii) $KA^2_{(a,b)}(C_p) = 4^{ab}q$.

Corollary 3.2 *If complete graph K_p with $p \geq 2$ is a $(p-1)$-regular graph, then*

(i) $KA^1_{(a,b)}(K_p) = 2^b q(p-1)^{ab}$;
(ii) $KA^2_{(a,b)}(K_p) = q(p-1)^{2ab}$.

Corollary 3.3 *If complete regular bipartite graph $K_{s,s}$ with $s \geq 1$ is a s-regular graph, then*

(i) $KA^1_{(a,b)}(K_{s,s}) = 2^b qs^{ab}$;
(ii) $KA^2_{(a,b)}(K_{s,s}) = qs^{2ab}$.

Corollary 3.4 *If n-hypercube graph Q_n is n-regular with 2^n vertices and $n2^{n-1}$ edges, then*

(i) $KA^1_{(a,b)}(Q_n) = 2^{b+n-1}n^{ab+1}$;
(ii) $KA^2_{(a,b)}(Q_n) = 2^{n-1}n^{2ab+1}$,

where the hypercube Q_n is the simple graph whose vertices are the n-tuples with entries in $0, 1$ and whose edges are the pairs of n-tuples that differ in exactly one position.

Corollary 3.5 *If G is generalized Petersen graph $GP(n,k)$ which is 3-regular with $2n$ vertices and $3n$ edges, then*

(i) $KA^1_{(a,b)}(G) = 2^b n3^{ab+1}$;
(ii) $KA^2_{(a,b)}(G) = n3^{2ab+1}$,

where the generalized Petersen graph denoted by $GP(n,k)$ for $n \geq 3$ and $1 \leq k \leq \lfloor (n-1)/2 \rfloor$ is a connected cubic graph consisting of an inner star polygon $\{n,k\}$ (circulant graph $Ci_n(k)$) and an outer regular polygon n (cycle graph C_n) with corresponding vertices in the inner and outer polygons connected with edges.

§4. Cartesian Product Graphs

According to Hammack et al. [14], the Cartesian products of graphs were defined in 1912 by Whitehead and Russel. They were repeatedly rediscovered later, notably by Sabidussi (1960) and independently by Vizing (1963). The cartesian product of two graphs G and H, denoted by $G\Box H$, is a graph with vertex set $V(G\Box H) = V(G) \times V(H)$, that is, the set $\{(g,h)/g \in G, h \in H\}$. The edge set of $G\Box H$ consists of all pairs $[(g_1,h_1),(g_2,h_2)]$ of vertices with $[g_1,g_2] \in E(G)$ and $h_1 = h_2$, or $g_1 = g_2$ and $[h_1,h_2] \in E(H)$.

4.1. Grid Graph

The $m \times n$ grid graph can be represented as a cartesian product of $P_m\Box P_n$ of a path of length $m-1$ and a path of length $n-1$. This grid graph is denoted by $G_{m,n}$ with (mn)-vertices and $(2mn-m-n)$-edges.

Theorem 4.1 *Let $G = G_{m,n}$ be an $m \times n$ grid graph. Then*

$$KA^1_{(a,b)}(G) = \begin{cases} 4\,(2^b\ 2^{ab}), & \text{if } m=n=2 \\ 2^{b(a+1)+1} & \\ +4(2^a+3^a)^b & \\ +(3n-8)2^b3^{ab}, & \text{if } m=2, n\geq 3 \\ 8(2^a+3^a)^b & \\ +2^{b+1}(m+n-6)3^{ab} & \\ +2(m+n-4)(3^a+4^a)^b & \\ +(2mn-5(m+n)+12)2^b4^{ab} & \text{if } m\geq 3, m\leq n. \end{cases}$$

$$KA^2_{(a,b)}(G) = \begin{cases} 4^{ab+1}, & \text{if } m=n=2 \\ 2.4^{ab}+4.6^{ab} & \\ +(3n-8)9^{ab}, & \text{if } m=2, n\geq 3 \\ 8.6^{ab}+2(m+n-6)9^{ab} & \\ +2(m+n-4)12^{ab} & \\ +(2mn-5(m+n)+12)16^{ab} & \text{if } m\geq 3, m\leq n. \end{cases}$$

and

$$KA^3_{(a,b)}(G) = \begin{cases} 0, & \text{if } m=n=2 \\ 4.|2^a-3^a|^b, & \text{if } m=2, n\geq 3 \\ 8.|2^a-3^a|^b & \\ +2(m+n-4)|3^a-4^a|^b & \text{if } m\geq 3, m\leq n. \end{cases}$$

Proof Let $G = G_{m,n}$ be an $m \times n$ grid graph with (mn)-vertices and $(2mn-m-n)$-edges. By algebraic method, we have

$m \times n$ grid	$(d_G(u), d_G(v))$	Number of edges
2×2	$(2, 2)$	4
$2 \times n$, $n \geq 3$	$(2, 2)$	2
	$(2, 3)$	4
	$(3, 3)$	$3n - 8$
$m \times n, m \leq n, m \geq 3$	$(2, 3)$	8
	$(3, 3)$	$2(m + n - 6)$
	$(3, 4)$	$2(m + n - 4)$
	$(4, 4)$	$2mn - 5(m + n) + 12$

Table 1 Degree partition of $G_{m,n}$.

By the definitions of (a, b)-KA indices and Table 1, on simplification, we have

Case 1. If $m = n = 2$, then

(i) $KA^1_{(a,b)}(G) = 4(2^b 2^{ab})$;
(ii) $KA^2_{(a,b)}(G) = 4^{ab+1}$;
(iii) $KA^3_{(a,b)}(G) = 0$.

Case 2. If $m = 2$ and $n \geq 3$, then

(i) $KA^1_{(a,b)}(G) = 2^{b(a+1)+1} + 4(2^a + 3^a)^b + (3n - 8)2^b 3^{ab}$;
(ii) $KA^2_{(a,b)}(G) = 2.4^{ab} + 4.6^{ab} + (3n - 8)9^{ab}$;
(iii) $KA^3_{(a,b)}(G) = 4.|2^a - 3^a|^b$.

Case 3. If $m \geq 3$ and $m \leq n$, then

(i) $KA^1_{(a,b)}(G) = 8(2^a + 3^a)^b + 2^{b+1}(m + n - 6)3^{ab} + 2(m + n - 4)(3^a + 4^a)^b + (2mn - 5(m + n) + 12)2^b 4^{ab}$;
(ii) $KA^2_{a,b}(G) = 8.6^{ab} + 2(m+n-6)9^{ab} + 2(m+n-4)12^{ab} + (2mn-5(m+n)+12)16^{ab}$;
(iii) $KA^3_{a,b}(G) = 8.|2^a - 3^a|^b + 2(m + n - 4)|3^a - 4^a|^b$.

Thus, the result follows. □

4.2. Torus Grid Graph

The Torus grid graph $T_{m,n}$ is the graph formed from the graph cartesian product $C_m \square C_n$ of the cycle graphs C_m and C_n. $C_m \square C_n$ is isomorphic to $C_n \square C_m$.

Theorem 4.2 *Let $G = T_{m,n}$ be a Torus grid graph which is 4- regular graph with mn vertices and $2mn$ edges. Then*

(i) $KA^1_{(a,b)}(G) = mn.2^{b+1}4^{ab}$;
(ii) $KA^2_{(a,b)}(G) = 2mn.16^{ab}$;
(iii) $KA^3_{(a,b)}(G) = 0$.

Proof Let $G = T_{m,n}$ be a Torus grid graph which is 4- regular graph with mn vertices and

$2mn$ edges.

(i) The first (a,b)-KA index is

$$\begin{aligned} KA^1_{(a,b)}(G) &= \sum_{uv\in E(G)} [d_G(u)^a + d_G(v)^a]^b \\ &= \sum_{uv\in E(G)} [4^a + 4^a]^b = q2^b4^{ab} = mn.2^{b+1}4^{ab}. \end{aligned}$$

(ii) The second (a,b)-KA index is

$$\begin{aligned} KA^2_{(a,b)}(G) &= \sum_{uv\in E(G)} [d_G(u)^a . d_G(v)^a]^b \\ &= \sum_{uv\in E(G)} [4^a.4^a]^b = q4^{2ab} = 2mn.16^{ab}. \end{aligned}$$

(iii) The third (a,b)-KA index is

$$\begin{aligned} KA^3_{(a,b)}(G) &= \sum_{uv\in E(G)} |d_G(u)^a - d_G(v)^a|^b \\ &= \sum_{uv\in E(G)} |4^a - 4^a|^b = 0. \end{aligned}$$

Thus, the result follows. □

4.3. Cylinder Grid Graph

The cylinder grid graph $C_{m,n}$ is the graph formed from the cartesian product $P_m \times C_n$ of the path graph P_m and the cycle graph C_n. That is, the cylinder grid graph consists of m copies of C_n represented by circles and n copies of P_m represented by paths transverse the m circles.

Theorem 4.3 *Let $G = C_{m,n}$ be a cylinder grid graph with $n \geq 3$. Then,*

$$KA^1_{(a,b)}(G) = \begin{cases} n2^b3^{ab+1}, & \text{if } m = 2 \\ n2^{b+1}3^{ab} + 2n(3^a + 4^a)^b & \\ +(2mn - 5n)2^b4^{ab}, & \text{if } m \geq 3. \end{cases}$$

$$KA^2_{(a,b)}(G) = \begin{cases} n3^{2ab+1}, & \text{if } m = 2 \\ 2n3^{2ab} + 2n3^{ab}4^{ab} & \\ +(2mn - 5n)4^{2ab}, & \text{if } m \geq 3. \end{cases}$$

and

$$KA^3_{(a,b)}(G) = \begin{cases} 0, & \text{if } m = 2 \\ 2n|3^a - 4^a|^b, & \text{if } m \geq 3. \end{cases}$$

Proof Let $G = C_{m,n}$ be a cylinder grid graph with mn vertices, where $n \geq 3$.

Case 1. If $m = 2$, then the graph G is 3-regular with $3n$ edges. Thus

(i) The first (a, b)-KA index is

$$\begin{aligned} KA^1_{(a,b)}(G) &= \sum_{uv\in E(G)} [d_G(u)^a + d_G(v)^a]^b \\ &= \sum_{uv\in E(G)} [3^a + 3^a]^b = q2^b3^{ab} = n2^b3^{ab+1}. \end{aligned}$$

(ii) The second (a, b)-KA index is

$$\begin{aligned} KA^2_{a,b}(G) &= \sum_{uv\in E(G)} [d_G(u)^a.d_G(v)^a]^b \\ &= \sum_{uv\in E(G)} [3^a.3^a]^b = q3^{2ab} = n3^{2ab+1}. \end{aligned}$$

(iii) The third (a, b)-KA index is

$$KA^3_{(a,b)}(G) = \sum_{uv\in E(G)} |d_G(u)^a - d_G(v)^a|^b = \sum_{uv\in E(G)} |3^a - 3^a|^b = 0.$$

Case 2. If $m \geq 3$, then by algebraic method, we have Table 2.

$(d_G(u), d_G(v))$	Number of edges
$(3, 3)$	$2n$
$(3, 4)$	$2n$
$(4, 4)$	$2mn - 5n$

Table 2 Degree partition of $C_{m,n}$ with $m \geq 3$.

By the definitions of (a, b)-KA indices and Table-2, on simplification, we have

(i) $KA^1_{(a,b)}(G) = n2^{b+1}3^{ab} + 2n(3^a + 4^a)^b + (2mn - 5n)2^b4^{ab}$.

(ii) $KA^2_{(a,b)}(G) = 2n3^{2ab} + 2n3^{ab}4^{ab} + (2mn - 5n)4^{2ab}$.

(iii) $KA^3_{(a,b)}(G) = 2n|3^a - 4^a|^b$.

Thus, the result follows. □

§5. Lollipop Graph

The (m, n)-lollipop graph is the graph obtained by joining a complete graph K_m to a path P_n with a bridge.

Theorem 5.1 *Let $G = LP(m,n)$ be a Lollipop graph. Then,*

$$KA^1_{(a,b)}(G) = \begin{cases} (1+m^a)^b \\ +(m-1)[(m-1)^a+m^a]^b \\ +2^b(m-1)^{ab}\Big(\dfrac{m^2-3m}{2}+1\Big), & \text{if } n=1,\ m\geq 3 \\ (1+2^a)^b+(n-1)2^{b(1+a)} \\ +3(2^a+3^a)^b, & \text{if } m=3, n\geq 2 \\ (1+2^a)^b+(n-2)2^{b(1+a)} \\ +(2^a+m^a)^b \\ +2^b(m-1)^{ab}\Big(\dfrac{m^2-3m}{2}+1\Big) \\ +(m-1)[(m-1)^a+m^a]^b, & \text{if } m\geq 4, n\geq 2. \end{cases}$$

$$KA^2_{(a,b)}(G) = \begin{cases} m^{ab}+m^{ab}(m-1)^{ab+1} \\ +(m-1)^{2ab}\Big(\dfrac{m^2-3m}{2}+1\Big), & \text{if } n=1,\ m\geq 3 \\ 2^{ab}+(n-1)4^{ab}+3.6^{ab}, & \text{if } m=3, n\geq 2 \\ 2^{ab}+(n-2)4^{ab}+2^{ab}m^{ab} \\ +(m-1)^{ab+1}m^{ab} \\ +(m-1)^{2ab}\Big(\dfrac{m^2-3m}{2}+1\Big), & \text{if } m\geq 4, n\geq 2. \end{cases}$$

and

$$KA^3_{(a,b)}(G) = \begin{cases} |1-m^a|^b \\ +(m-1)|(m-1)^a-m^a|^b, & \text{if } n=1,\ m\geq 3 \\ |1-2^a|^b+3|2^a-3^a|^b, & \text{if } m=3, n\geq 2 \\ |1-2^a|^b+|2^a-m^a|^b \\ +(m-1)|(m-1)^a-m^a|^b, & \text{if } m\geq 4, n\geq 2. \end{cases}$$

Proof Let $G = LP(m,n)$ be a Lollipop graph.

Case 1. If $n=1, m\geq 3$, then by algebraic computations, we have

$(d(u),d(v))$	Number of edges
$(1,m)$	1
$(m-1,m-1)$	$\dfrac{m^2-3m}{2}+1$
$(m-1,m)$	$m-1$

Table 3 Degree partition of $L(m,n)$ with $n=1, m\geq 3$.

By the definitions of (a,b)-KA indices and Table-3, on simplification, we have

(*i*) $KA^1_{(a,b)}(G) = (1+m^a)^b+(m-1)[(m-1)^a+m^a]^b+2^b(m-1)^{ab}\Big(\dfrac{m^2-3m}{2}+1\Big).$

(ii) $KA^2_{(a,b)}(G) = m^{ab} + m^{ab}(m-1)^{ab+1} + (m-1)^{2ab}\Big(\frac{m^2-3m}{2}+1\Big).$

(iii) $KA^3_{(a,b)}(G) = |1-m^a|^b + (m-1)|(m-1)^a - m^a|^b.$

Case 2. If $m = 3, n \geq 2$, then by algebraic computations, we have

$(d(u), d(v))$	Number of edges
$(1,2)$	1
$(2,2)$	$n-1$
$(2,3)$	3

Table 4 Degree partition of $L(m,n)$ with $m = 3, n \geq 2$.

By the definitions of (a,b)-KA indices and Table-4, on simplification, we have

(i) $KA^1_{(a,b)}(G) = (1+2^a)^b + (n-1)2^{b(1+a)} + 3(2^a+3^a)^b.$

(ii) $KA^2_{(a,b)}(G) = 2^{ab} + (n-1)4^{ab} + 3.6^{ab}.$

(iii) $KA^3_{(a,b)}(G) = |1-2^a|^b + 3|2^a - 3^a|^b.$

Case 3. If $m \geq 4, n \geq 2$, then by algebraic computations.

$(d(u), d(v))$	Number of edges
$(1,2)$	1
$(2,2)$	$n-2$
$(2,m)$	1
$(m-1, m-1)$	$\frac{m^2-3m}{2}+1$
$(m-1, m)$	$m-1$

Table 5 Degree partition of $L(m,n)$ with $m \geq 4, n \geq 2$.

By the definitions of (a,b)-KA indices and Table-5, on simplification, we have

(i) $KA^1_{(a,b)}(G) = (1+2^a)^b + (n-2)2^{b(1+a)} + (2^a+m^a)^b + 2^b(m-1)^{ab}\Big(\frac{m^2-3m}{2}+1\Big) + (m-1)[(m-1)^a + m^a]^b.$

(ii) $KA^2_{(a,b)}(G) = 2^{ab} + (n-2)4^{ab} + 2^{ab}m^{ab} + (m-1)^{ab+1}m^{ab} + (m-1)^{2ab}\Big(\frac{m^2-3m}{2}+1\Big).$

(iii) $KA^3_{(a,b)}(G) = |1-2^a|^b + |2^a - m^a|^b + (m-1)|(m-1)^a - m^a|^b.$

Thus the result follows. □

§6. Harary Graph

In 1962, Harary [13] introduced the Harary graph, which has maximum connectivity; therefore, it plays an important role in designing networks. This is a k-connected graph on p vertices of degree at least k with $\left\lceil \frac{kp}{2} \right\rceil$ edges. The Harary graph $H_{k,p}$ is constructed as follows:

1. *k even:* Let $k = 2r$. Then $H_{2r,p}$ is constructed by the vertices $0, 1, \ldots, p-1$ and two vertices i and j are joined if $i - r \leq j \leq i + r$.

2. *k odd, p even.* Let $k = 2r + 1$. Then $H_{2r+1,p}$ is constructed by first drawing $H_{2r,p}$ and then adding edges joining vertex i to vertex $i + (\frac{p}{2})$ for $1 \leq i \leq \frac{p}{2}$.

3. *k odd, p odd :* Let $k = 2r+1$. Then $H_{2r+1,p}$ is constructed by first drawing $H_{2r,p}$ and then adding edges joining vertex 0 to vertices $\frac{(p-1)}{2}$ and $\frac{(p+1)}{2}$ and vertex i to vertex $i + \frac{(p+1)}{2}$ for $1 \leq i \leq \frac{(p-1)}{2}$.

Theorem 6.1 *Let $G = H_{k,p}$ be a Harary graph.*

(1) *If k is even, then*

(i) $KA^1_{(a,b)}(G) = \left\lceil \frac{kp}{2} \right\rceil 2^b k^{ab}$;
(ii) $KA^2_{(a,b)}(G) = \left\lceil \frac{kp}{2} \right\rceil k^{2ab}$;
(iii) $KA^3_{(a,b)}(G) = 0$.

(2) *If k is odd and p is even, then*

(i) $KA^1_{(a,b)}(G) = \left\lceil \frac{kp}{2} \right\rceil 2^b k^{ab}$;
(ii) $KA^2_{(a,b)}(G) = \left\lceil \frac{kp}{2} \right\rceil k^{2ab}$;
(iii) $KA^3_{(a,b)}(G) = 0$.

(3) *If k is odd and p is odd, then*

(i) $KA^1_{(a,b)}(G) = \left\{ \left\lceil \frac{kp}{2} \right\rceil - (k+1) \right\} (2^b k^{ab}) + (k+1)(k^a + (k+1)^a)^b$;
(ii) $KA^2_{(a,b)}(G) = \left\{ \left\lceil \frac{kp}{2} \right\rceil - (k+1) \right\} (k^{2ab}) + (k+1)(k^{ab}(k+1)^{ab})$;
(iii) $KA^3_{(a,b)}(G) = (k+1)|k^a - (k+1)^a|^b$.

Proof Let $G = H_{k,p}$ be a Harary graph. We have

(1) If k is even, then

(i) The first (a, b)-KA index is

$$\begin{aligned} KA^1_{(a,b)}(G) &= \sum_{uv \in E(G)} [d_G(u)^a + d_G(v)^a]^b \\ &= \sum_{uv \in E(G)} [k^a + k^a]^b = q2^b k^{ab} = \left\lceil \frac{kn}{2} \right\rceil 2^b k^{ab}. \end{aligned}$$

(ii) The second (a, b)-KA index is

$$\begin{aligned} KA^2_{(a,b)}(G) &= \sum_{uv \in E(G)} [d_G(u)^a . d_G(v)^a]^b \\ &= \sum_{uv \in E(G)} [k^a . k^a]^b = qk^{2ab} = \left\lceil \frac{kn}{2} \right\rceil k^{2ab}. \end{aligned}$$

(iii) The third (a,b)-KA index is

$$\begin{aligned} KA^3_{(a,b)}(G) &= \sum_{uv\in E(G)} |d_G(u)^a - d_G(v)^a|^b \\ &= \sum_{uv\in E(G)} |k^a - k^a|^b = 0. \end{aligned}$$

(2) If k is odd and p is even, then

(i) The first (a,b)-KA index is

$$\begin{aligned} KA^1_{(a,b)}(G) &= \sum_{uv\in E(G)} [d_G(u)^a + d_G(v)^a]^b \\ &= q2^bk^{ab} = \left\lceil \frac{kn}{2} \right\rceil 2^bk^{ab}. \end{aligned}$$

(ii) The second (a,b)-KA index is

$$\begin{aligned} KA^2_{(a,b)}(G) &= \sum_{uv\in E(G)} [d_G(u)^a.d_G(v)^a]^b \\ &= qk^{2ab} = \left\lceil \frac{kn}{2} \right\rceil k^{2ab}. \end{aligned}$$

(iii) The third (a,b)-KA index is

$$KA^3_{(a,b)}(G) = \sum_{uv\in E(G)} |d_G(u)^a - d_G(v)^a|^b = \sum_{uv\in E(G)} |k^a - k^a|^b = 0.$$

(3) If k is odd and p is odd, then

(i) The first (a,b)-KA index is

$$\begin{aligned} KA^1_{(a,b)}(G) &= \sum_{uv\in E(G)} [d_G(u)^a + d_G(v)^a]^b \\ &= \left\{ \left\lceil \frac{kp}{2} \right\rceil - (k+1) \right\} (k^a + k^a)^b + (k+1)[k^a + (k+1)^a]^b \\ &= \left\{ \left\lceil \frac{kp}{2} \right\rceil - (k+1) \right\} (2^bk^{ab}) + (k+1)[k^a + (k+1)^a]^b. \end{aligned}$$

(ii) The second (a,b)-KA index is

$$\begin{aligned} KA^2_{(a,b)}(G) &= \sum_{uv\in E(G)} [d_G(u)^a.d_G(v)^a]^b \\ &= \left\{ \left\lceil \frac{kp}{2} \right\rceil - (k+1) \right\} (k^a.k^a)^b + (k+1)[k^a.(k+1)^a]^b \\ &= \left\{ \left\lceil \frac{kp}{2} \right\rceil - (k+1) \right\} (k^{2ab}) + (k+1)[k^{ab}(k+1)^{ab}]. \end{aligned}$$

(iii) The third (a,b)-KA index is

$$\begin{aligned} KA^3_{(a,b)}(G) &= \sum_{uv\in E(G)} |d_G(u)^a - d_G(v)^a|^b \\ &= \left\{\left\lceil \frac{kp}{2} \right\rceil - (k+1)\right\} |k^a - k^a|^b + (k+1)|k^a - (k+1)^a|^b \\ &= (k+1)|k^a - (k+1)^a|^b. \end{aligned}$$

Thus, the result follows. □

§7. Conclusions

Being new generalized version of vertex degree based topological indices, the (a,b) KA-indices lies on the fact that their special cases, for pertinently chosen values of the parameters a and b, coincide with the vast majority of previously considered topological indices. For the comparative advantages, applications and in mathematical point of view, few problems are suggested by this research, among them are the following.

Problem 7.1 *Find the extremal values and extremal graphs of the* (a,b)*-KA indices.*

Problem 7.2 *Find the values of* (a,b)*-KA indices for certain classes of chemical graphs and explore some results towards QSPR / QSAR / QSTR Model.*

Problem 7.3 *Obtain the relationship between* (a,b)*-KA indices in terms of other degree/ distance/spectral based topological indices.*

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